CODE	3VHA (PDB)	Resolution	1.4
Name		Ring size	16
Formula	C21H21N3O2S	# Ligand atoms	27
Type	MACROCYCLE	Scorpion Score	12.1

Mol. Weight (Da)	379.48	Saturated/ Unsaturated	U
cLogP	5.5772		
tPSA	69.2	Chiral centres.ring	0
#HBD's	2	Chiral centres.sub	0
#HBA's	5		
$N_{RB\ (RING)}$	10	$N_{RB\ (SUBSTITUENT)}$	0

Number of substituents	3	P/NP balance, substituents	3/8
Large (≥5HA)	-	P/NP balance, peripheral groups	-
Small (2-4HA)	3		
Proportion HA in substituents	41%	Degrees of unsaturation ring	13
Number of peripheral groups	-	N:O ratio	3:2
		Chiral centres	0

Polarity distribution ligand atoms

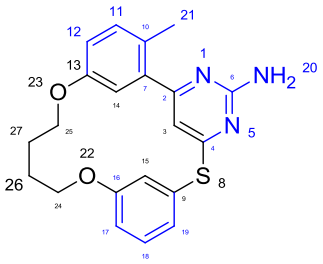
	All		Contact	
	Polar	*Nonpolar*	*Polar*	*Nonpolar*
Ring	3	13	1	4
Substituent	3	8	3	3
Peripheral groups	-	-		
Total	6	21	-	-

Protein name	HSP90
Organism	Homo sapiens
Classification	Chaperone/ inhibitor
Binding mode	Compact
Receptor secondary structure topology	
Number of residue 'hotspots'	12

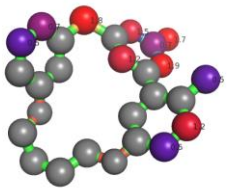
Number of protein-ligand interactions* ('Database link')

Hydrogen bond	1	Hydrogen donor-π	-
Ionic interaction	-	π-π	-
Cation-dipole	-	VdW interaction	14
Cation-π	-	Unfavourable	-
Dipolar interaction	-	Poor-angle	3
Halogen bond	-	Unclassified	
Water-mediated interaction	3		

2D-STRUCTURE LIGAND



3D-STRUCTURE LIGAND +SCORPIONSCORE ('Scorpion link')

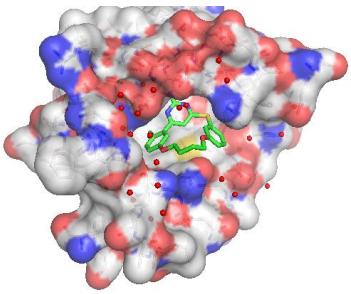


Physicochemical properties

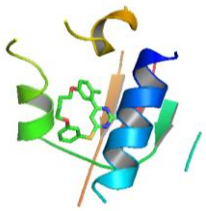
'click for publication'

IC_{50}	HCT 116	5.5
IC_{50}	NCI- N87	3.8

LIGAND-PROTEIN COMPLEX (I) ('Pymol link')



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis